

Reply to the comment of T.Gilbert and D.P.Sanders on “Capturing correlations in chaotic diffusion by approximation methods”

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This is a reply to the comment by Gilbert and Sanders [arXiv:1111.6271 (2011)]. We point out that their comment is a follow-up of a previous discussion which we briefly summarize before we refute their new criticism.

In their comment [1] Gilbert and Sanders argue that our application of persistent random walk theory to maps [2], in response to their reference [3], is ‘inaccurate’, due to a ‘misinterpretation’ of simple random walk theory, and ‘based on a confusion between two different time scales’. Their comment is a follow-up of a discussion that has started with [4] authored by one of us. This work was already criticized by Gilbert and Sanders in [3] on which we responded with [2]. We welcome the opportunity to briefly summarize this discussion in order to put the present comment by Gilbert and Sanders into context before we refute their new criticism.

In [4] the Taylor-Green-Kubo formula, which expresses the diffusion coefficient in terms of the velocity autocorrelation function, has been worked out for periodic particle billiards by mapping the time-continuous dynamics onto a time-discrete correlated random walk on a periodic lattice. This approach expresses the diffusion coefficient in the form of a series expansion that converges exactly. Calculating the k -th order terms of this expansion yields a systematic approximation procedure for the diffusion coefficient. Non-trivial information is provided by this method in form of the parameter dependence of the convergence, as was demonstrated in [4] for one-dimensional maps and for billiards both numerically and analytically. This conceptually trivial method was successfully applied to a number of different dynamical systems in order to physically understand the irregular parameter dependence of diffusion coefficients, see [5] and further references therein.

In a first round of criticism Gilbert and Sanders argued that this method is mathematically wrong and physically meaningless [3]. They claimed that in order to obtain ‘accurate results’ for capturing correlations one must use persistent random walk theory. A substantial part of this theory was originally developed for correlated random walks on lattices (see, e.g., [6, 7] and further references therein). By employing the Taylor-Green-Kubo formalism of [4], Gilbert and Sanders adapted this theory to billiards and demonstrated its application by numerical results [3].

This criticism of Gilbert and Sanders was refuted in [2] by analyzing diffusion in a simple one-dimensional

chaotic map. This model had the advantage that in contrast to billiards it is amenable to rigorous analysis. Here both the Taylor-Green-Kubo approximation method of [4] and a suitable adaption of persistent random walk theory to maps (plus another new, third method) were applied and compared with each other. Our results reconfirmed that the criticism by Gilbert and Sanders was unfounded, as could already have been inferred from [4, 5] and further references therein. The present comment by Gilbert and Sanders on [2] does not contain any further evidence that this approach is incorrect. We are thus pleased to conclude that Gilbert and Sanders have accepted the invalidity of their previous criticism published in [3].

Instead, with their comment [1] Gilbert and Sanders launch a second round of criticism on a new aspect that is still related to the Taylor-Green-Kubo formalism but different from the previously criticized approximation method. Their argument is summarized as follows: Transposing persistent random walk theory to billiards on the basis of [4] led to a correlated random walk dynamics which did not incorporate a probability that particles on the random walk lattice remain at a site [3]. The new criticism of Gilbert and Sanders is that, by working out persistent random walk theory for time-discrete maps defined on a periodic lattice, we included a non-zero probability that particles remain on a site. In view of their own adaption of persistent random walk theory to billiards [3], which motivated [2], they argued that we have ‘confused’ two different time scales in our analysis, namely ‘the average time spent by a walker at any given site before it moves on to a neighboring one’ with the ‘unit time scale of the underlying process’.

Our reply to their criticism is as follows: We first emphasize that persistent random walk theory has to a large extent originally been developed for time-discrete stochastic random walks on periodic lattices [6, 7]. The one-dimensional map studied in [2] is a simple deterministic realization of such a random walk. Gilbert and Sanders’s reference [3] suggests a suitable adaption of persistent random walk theory to billiards. In their comment they now insist that their billiard version must be re-transposed to maps by ruling out any non-zero probability that a walker remains on a site. This constraint is at variance with original persistent random walk theory, which explicitly does incorporate such probabilities [6], as motivated by applying this theory to experimental data [8]. Furthermore, in a follow-up article [9] Gilbert et

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al. reproduce results that are contained as a special case in a more general formula derived in [6], which incorporates a non-zero probability that a walker remains on a site, compare Eqs.(1.3) and (5.4) in [6] with (2.17) in [9]. Our results for maps [2] are consequently neither ‘inaccurate’, nor is there any ‘flaw’ in view of standard persistent random walk theory. Secondly, there is no ‘misunderstanding of the Machta-Zwanzig approximation’, i.e., simple uncorrelated random walk theory for billiards [5]: As was shown in [2], this approximation is exactly reproduced by our method for our model, cf. Eq.(26). In summary, there is neither any contradiction between persistent random walk theory and how we apply it to maps, nor is there any error in our theory, in contrast to what Gilbert and Sanders suggest in their comment.

We finally address the criticism of Gilbert and Sanders of having ‘confused’ two different time scales: A key observation in [4] was that the natural time scale in order to map time-continuous diffusion in billiards onto a time-discrete random walk on a periodic lattice is the average escape time τ of a particle to move from one fundamental cell to another. For time-discrete diffusion on periodic lattices, as for time-discrete maps, the natural time scale is the unit time, possibly multiplied by some factor. It is thus convenient to choose these natural time scales for working out persistent random walk theory in these different systems, and there is no inaccuracy in doing so. Another important point is that in [2] we compare three different approximation schemes for diffusion with each other. In order to provide a fair comparison between these different methods, one needs to set them up by using the very same time scale. Persistent random walk theory and the Taylor-Green-Kubo approximation method are based on the very same Taylor-Green-Kubo formula, which guarantees that this condition is fulfilled

by default. In [2] we have conveniently chosen the unit time as a time scale therein. Hence, instead of any confusion, there was deliberately a clear choice of a unique time scale. The comment by Gilbert and Sanders shows that by using the average escape time τ for maps instead of unit time, the textbook uncorrelated random walk result matches to the lowest order of persistent random walk theory with zero probability of trapping. We encourage Gilbert and Sanders to go beyond this lowest order by re-calculating our *higher-order corrections* for *all three approximation methods* [2] using a non-integer time scale τ for time-discrete maps.

We conclude our reply by pointing out that, as Gilbert and Sanders have already misread [3] the Taylor-Green-Kubo approximation scheme developed in [4], they have also misread [1] reference [2]: Nowhere in our article do we suggest that there is ‘a serious limitation of [Gilbert and Sanders’s] formalism’ [3] due to zero velocity states. Such states merely prevented us from obtaining an analytical solution for the two-step approximation of our model, cf. the very last sentence in the Appendix of [2], a problem that was resolved by reverting to numerical methods. The comment by Gilbert and Sanders is thus motivated by an inadequate interpretation of our article. A correct account is that we have compared three different approximation methods in it by applying them on the same footing, i.e., by using the very same fundamental time scale, to a given map. For this model we conclude that all these schemes have their own virtues and deficiencies. We thus repeat again, as we concluded already in [2], that we find ‘the quest for a unique way to approximate the diffusion coefficient of a dynamical system’, as repeatedly suggested by Gilbert and Sanders by pointing towards their own adaption of persistent random walk theory to billiards, ‘unnecessarily restrictive’.

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